

An Angular Multigrid Acceleration Method for S_N Equations with Highly Forward-Peaked Scattering

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Abstract

The angular multigrid method, previously developed for the acceleration of one-dimensional slab geometry S_N equations with highly forward-peaked scattering, is extended to multidimensional geometries. Analysis and testing shows that a straightforward extension to these geometries is unstable. However, we apply a diffusive filter to the multigrid corrections to create a modified method that is stable and effective for the acceleration of highly forward-peaked scattering transport iterations in multidimensional geometries.

1 Introduction

Many transport problems are characterized by highly forward-peaked anisotropic scattering. Such problems include, for example, the transport of charged particles such as ions and electrons. In these problems the Legendre expansion of the scattering cross section consists of numerous scattering moments of comparable magnitude; the magnitude decreases slowly as a function of cross section order. In particular, many physical cross sections are closely approximated by the Fokker-Planck cross section expansion (Pomraning, 1992).

The approximate solution of such problems by the discrete ordinates (S_N) method can be difficult to obtain due to the ineffectiveness of standard acceleration schemes. For example, the diffusion synthetic acceleration (DSA) method, which accelerates the zeroth (Larsen, 1984) or the zeroth and first (Morel, 1982) flux moments, yields at best an iterative spectral radius of unity in the limit of highly forward-peaked scattering. The ineffectiveness of these methods for such problems stems from the fact that many of the higher order moments of the iterative error are not significantly attenuated by source iteration. Thus an effective acceleration scheme must calculate corrections for these higher order error modes.

One acceleration scheme that has been found to be effective for highly forward-peaked scattering in one-dimensional slab geometry is the angular multigrid (ANMG) method (Morel, 1991). In this scheme a high order S_N calculation is accelerated by a series of increasingly lower order transport sweeps and then by DSA as the final step. At each step the cross sections are manipulated so that the corresponding transport sweep provides good attenuation of the moments that are not accelerated by lower order steps; the net effect is effective acceleration of modes of all orders. In this paper we extend the angular multigrid method to multidimensional transport problems.

2 The Multidimensional Angular Multigrid Method

Before defining the general angular multigrid method for multidimensional S_N calculations of arbitrary order, we will first describe its application to an S_8 calculation. The ANMG scheme for S_8 calculations is a four-grid scheme:

1. Perform a transport sweep for the S_8 equations.
2. Perform a transport sweep for the S_4 equations with a P_4 (or P_5) expansion for the S_8 residual as the inhomogeneous source. The order of the expansion depends on the dimensionality of the problem and is a consequence of the fact that a Galerkin quadrature (Morel, 1989) must be used.
3. Perform a transport sweep for the S_2 equations with a P_2 (or P_3) expansion for the S_4 residual as the inhomogeneous source.
4. Solve the diffusion equation with a P_0 expansion for the S_2 residual as the inhomogeneous source.
5. Apply a diffusive filter to the corrections from steps 2 and 3.
6. Add the corrections from steps 4 and 5 to the Legendre moments of the S_8 iterate to obtain the accelerated S_8 moments.

The above scheme differs somewhat from the slab geometry ANMG scheme. In step 4 above we use the standard DSA scheme that accelerates only the zeroth moment, since it has been shown that the DSA scheme that accelerates both the zeroth and first moments is unstable in multidimensional geometries for highly forward-peaked scattering (Adams, 1993). We compensate for the loss of a more effective DSA scheme by using an S_2 sweep as the lowest order transport sweep, whereas the original ANMG scheme uses an S_4 sweep as its lowest order sweep. In step 5 we apply a diffusive filter to the corrections from the lower order transport sweeps. This filtering step is necessary because our analysis (described in the next section) shows that without it the ANMG scheme amplifies rather than damps high-frequency error modes. The diffusion operator is known to smooth such modes, and we take advantage of that property here. Finally, note the use of Galerkin quadratures and cross section expansions of higher order than is standard. The necessity of their use is shown in a companion paper in these proceedings (Pautz, 1999).

The equations corresponding to the steps above are:

$$[\mathbf{\Omega} \cdot \mathbf{\nabla} + \sigma_t]_8 \Psi_8^{(l+\frac{1}{2})} = M_8 \Sigma_8 \Phi_8^{(l)} + q, \quad (1a)$$

$$\Phi_8^{(l+\frac{1}{2})} = D_8 \Psi_8^{(l+\frac{1}{2})}, \quad (1b)$$

$$[\mathbf{\Omega} \cdot \mathbf{\nabla} + \sigma_t]_4 \Psi_4^{(l)} = M_4 P_{8 \rightarrow 4} \Sigma_8 \left(\Phi_8^{(l+\frac{1}{2})} - \Phi_8^{(l)} \right), \quad (1c)$$

$$\Phi_4^{(l)} = D_4 \Psi_4^{(l)}, \quad (1d)$$

$$[\mathbf{\Omega} \cdot \mathbf{\nabla} + \sigma_t]_2 \Psi_2^{(l)} = M_2 P_{4 \rightarrow 2} \Sigma_4 \left(\Phi_4^{(l)} \right), \quad (1e)$$

$$\Phi_2^{(l)} = D_2 \Psi_2^{(l)}, \quad (1f)$$

$$\left[-\nabla \cdot \frac{1}{3\sigma_{t,2}} \nabla + \sigma_a \right] f_0^{(l)} = P_{2 \rightarrow 0} \Sigma_2 \Phi_2^{(l)}, \quad (1g)$$

$$\left[-\nabla \cdot \frac{\alpha_f}{3\sigma_f} \nabla + \sigma_f \right] \mathbf{f}_{corr}^{(l)} = \sigma_f \left[\Phi_4^{(l)} + P_{2 \rightarrow 4} \Phi_2^{(l)} \right], \quad (1h)$$

$$\Phi_8^{(l+1)} = \Phi_8^{(l+\frac{1}{2})} + P_{4 \rightarrow 8} \mathbf{f}_{corr}^{(l)} + P_{0 \rightarrow 8} f_0^{(l)}, \quad (1i)$$

where M_N and D_N are the moments-to-discrete and discrete-to-moments matrices for the N th-order quadrature set, Σ_N is the scattering cross section matrix at level N , $P_{N \rightarrow N'}$ is the restriction (prolongation) operator from level N to level N' , σ_f is the filter cross section, and α_f is the filter tuning parameter. The remaining quantities are defined in the original angular multigrid paper (Morel, 1991).

The effectiveness of the ANMG scheme depends on how well it attenuates the highest order moments at each level. To increase the attenuation we use the extended transport correction (Lathrop, 1965) at each level. In the extended transport correction we subtract a constant from all scattering cross section moments:

$$\sigma_n^* = \sigma_n - \sigma_{corr}, \quad n \leq L. \quad (2)$$

where L is the expansion order. If the Galerkin quadrature is used, the above “correction” has no effect on the converged solution at any level, but it will alter the rate of iterative convergence (Morel, 1991). The invariance of the solution can be seen by taking moments of the discrete-ordinates transport equations to produce an equivalent set of equations for angular moments. In these equations the σ_{corr} term cancels out and thus has no effect on the solution. We choose σ_{corr} such that the upper half of the moments at any level are attenuated as much as possible.

In the general ANMG scheme an S_N calculation is accelerated by an $S_{N'}$ sweep, in which $N' = Half(N)$, where

$$Half(N) = \begin{cases} \frac{N}{2}, & \frac{N}{2} \text{ even} \\ \frac{N}{2} + 1, & \frac{N}{2} \text{ odd} \end{cases}. \quad (3)$$

The $S_{N'}$ sweep is in turn accelerated by a transport sweep of order $Half(N')$. This process continues through successively lower transport sweep orders; the final steps are an S_2 sweep, DSA, filtering of the sweep corrections, and adding of the corrections to the S_N flux iterates.

3 Fourier Analysis

In order to determine the effectiveness and stability of the ANMG scheme we perform a series of Fourier analyses. We examine an infinite, homogeneous medium in two-dimensional Cartesian geometry and subtract Eqs. (1) from the analogous equations for the converged solution; this produces equations that are satisfied by iteration errors. We assume that the error in a given iterate can be decomposed into modes of the form $e^{i\boldsymbol{\lambda} \cdot \mathbf{r}}$, where \mathbf{r} is the spatial location and $\boldsymbol{\lambda}$ is the wave number of a particular Fourier mode. We substitute this ansatz into the equations satisfied by the iteration errors and obtain an eigenvalue problem. The set of eigenvalues obtained for each $\boldsymbol{\lambda}$ determines the rate at

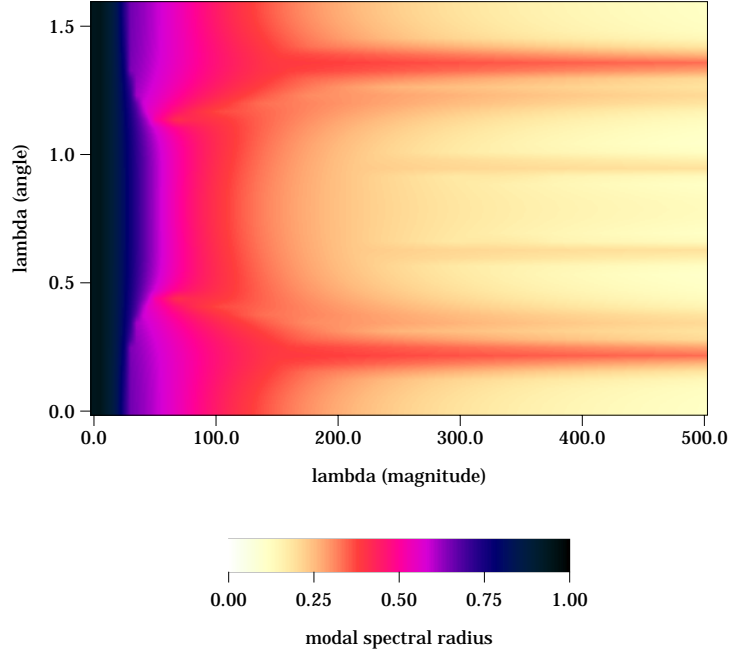


Figure 1: Fourier analysis of S_8 -DSA iteration, optimized Fokker-Planck scattering.

which errors will be attenuated or grow. For an iterative scheme to be stable the absolute value of all eigenvalues for all λ must be less than unity; for an iterative scheme to be effective their magnitudes must be bounded well below unity.

To demonstrate the use of Fourier analyses and to show the need for the ANMG acceleration scheme we examine the spatially analytic S_8 equations with source iteration and DSA applied to a medium with Fokker-Planck (FP) scattering and no absorption. The FP scattering kernel closely approximates many physical forward-peaked cross sections; it is given by

$$\sigma_n = \frac{\sigma_{tr}}{2} [L(L-1) - n(n+1)], \quad (4)$$

where σ_{tr} is the transport (or momentum transfer) cross section (Morel, 1981). In Figure 1 we plot the eigenvalue of greatest magnitude for each Fourier mode (the modal spectral radius) for this problem; $|\lambda|$ is measured in transport mean free paths. Note that the high frequency modes are relatively well attenuated by this iteration, whereas the low frequency modes are barely attenuated at all. The overall spectral radius σ for this iteration is 0.97, which is fairly close to unity. (The spectral radius is the maximum of all modal spectral radii.)

In Figure 2 we plot the results of the Fourier analysis for the ANMG accelerated S_8 scheme in which we neglect to filter the corrections as in Eq. (1h) and instead add the unfiltered corrections directly to the flux iterates. Although the low frequency modes are well attenuated now, we have introduced instabilities in some high frequency modes. That is, this iterative method diverges for the model problem.

We now see the motivation for diffusively filtering the corrections. As shown in Figure 1, the high frequency modes are relatively well attenuated by source iteration alone; they do not need any corrections from the ANMG scheme. However, low frequency modes are well attenuated by the ANMG

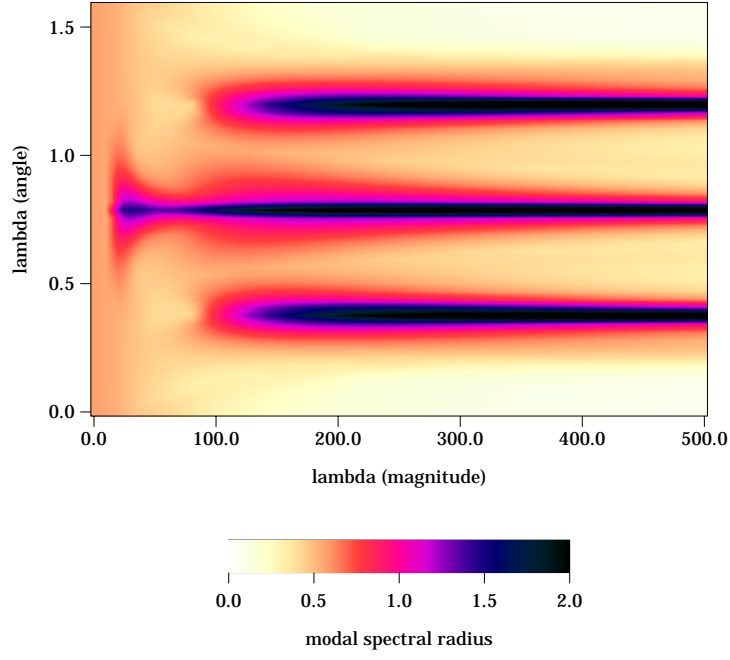


Figure 2: Fourier analysis of S_8 - S_4 - S_2 -DSA iteration, optimized FP scattering.

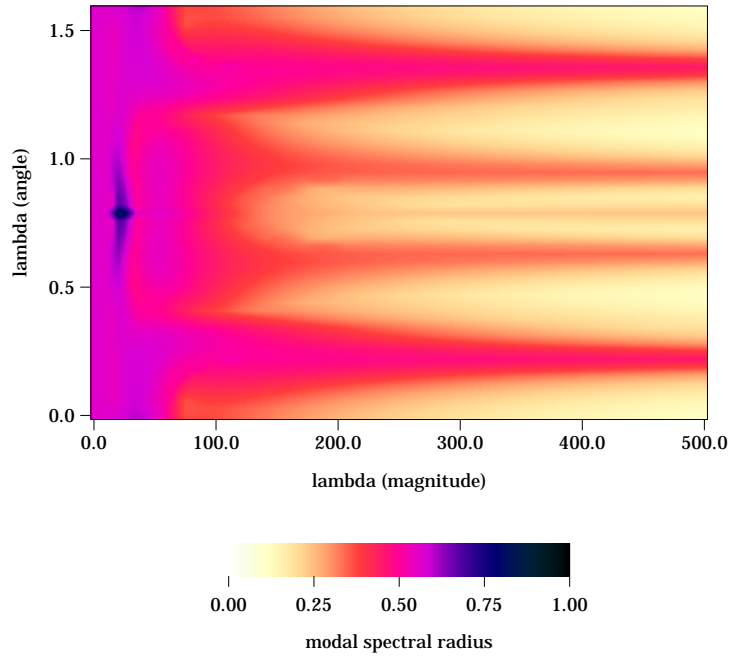


Figure 3: Fourier analysis of S_8 - S_4 - S_2 -DSA-filter iteration, optimized FP scattering ($\alpha_f = 1, \sigma_f = \sigma_{t,8}$).

scheme. In order to keep the ANMG corrections at low frequencies but to discard them at high frequencies we “filter” them with a diffusion operator. Consider the solution of a diffusion problem with a source of wave number λ :

$$\left[-\nabla \cdot \frac{\alpha}{3\sigma} \nabla + \sigma \right] F e^{i\lambda \cdot \mathbf{r}} = \sigma A e^{i\lambda \cdot \mathbf{r}}. \quad (5)$$

Given an input amplitude A , the “diffusively filtered” amplitude is:

$$F = A\sigma \left[\frac{\alpha}{3\sigma} \lambda^2 + \sigma \right]^{-1} = A \left[1 + \frac{\alpha \lambda^2}{3\sigma} \right]^{-1}. \quad (6)$$

Modes with large enough $|\lambda|$ (high frequency) are strongly attenuated while low-frequency modes are not. A small value of the “filter cross section” σ_f will increase the attenuation, whereas a large value will cause only very high frequency modes to be attenuated. In Figure 3 we plot the results of the Fourier analyses of the filtered ANMG scheme in which we have arbitrarily chosen $\alpha_f = 1$ and $\sigma_f = \sigma_{t,8}$. This iteration is stable and effective; the spectral radius is 0.85.

In Tables 1 and 2 we list the spectral radius for filtered ANMG schemes applied to transport calculations of various orders using a filter tuning parameter of unity and a filter cross section equal to the total cross section and to the transport cross section, respectively. The total cross section does not make a good filter cross section for calculations of general order. The total cross section of a Fokker-Planck kernel increases in magnitude as the order of the calculation is increased, thus increasing the range of frequencies allowed to pass through the filter, which at high enough orders permits instabilities to reappear. Although we could stabilize this scheme for any fixed calculation order by increasing the value of α_f , no fixed value of the filter tuning parameter will stabilize calculations of arbitrary order when the total cross section is used as the filter cross section. However, the transport cross section remains constant as the scattering order is increased, and as Table 2 shows it appears to work well as a filter cross section when $\alpha_f = 1$. We have not attempted to optimize the value of α_f . We note that the spectral radii obtained by the ANMG method can still be somewhat large for high-order quadrature sets, but they are much better than those obtained by the use of DSA alone.

We have also performed Fourier analyses of the ANMG scheme applied to spatially discrete S_N equations. We report here the results of the analyses of the bilinear discontinuous (BLD) finite element method on rectangles (Adams, 1991), with the DSA method of Wareing, Larsen, and Adams (WLA) (Wareing, 1991), as modified by Wareing (Wareing, 1999) as a DSA and filter operator. In spatially discrete Fourier analyses we obtain a spectral radius for each set of values of rectangle dimensions. Results for the S_8 ANMG scheme without and with filtering are shown in Tables 3 and 4, respectively. For optically thin cells we observe that the unfiltered scheme is unstable, as it was in the spatially analytic case, whereas the filtered scheme is stable. (We remark that the relatively large spectral radii for cells with high aspect ratios are caused by the particular DSA discretization (WLA) used and not by the ANMG part of the iteration. The WLA DSA discretization is known to degrade in this way, even for problems with isotropic scattering.) However, for cells of moderate or large optical thickness the ANMG scheme is stable whether or not filtering is applied. The reason that the method is stable for thicker cells even without filtering is that there is an upper limit on the frequency of error modes that can be supported in spatially discrete problems; potentially unstable modes simply do not exist if the cells are sufficiently thick.

Table 1: Spectral Radii of Filtered S_N -ANMG Iterations ($\alpha_f = 1, \sigma_f = \sigma_{t,N}$)

N	σ
4	0.65
6	0.63
8	0.85
10	0.95
12	1.04
14	1.32

Table 2: Spectral Radii of Filtered S_N -ANMG Iterations ($\alpha_f = 1, \sigma_f = \sigma_{tr}$)

N	σ
4	0.70
6	0.81
8	0.86
10	0.90
12	0.92
14	0.94

Table 3: Fourier Analysis Results, BLD S_8 - S_4 - S_2 -DSA (WLA) Iteration, Optimized FP Scattering

$\sigma_{tr} \Delta x$	$\sigma_{tr} \Delta y$		
	.01	1	100
.01	1.53		
1	0.64	0.64	
100	0.99	0.98	0.71

Table 4: Fourier Analysis Results, BLD S_8 - S_4 - S_2 -DSA-filter (WLA) Iteration, Optimized FP Scattering, ($\alpha_f = 1, \sigma_f = \sigma_{t,8}$)

$\sigma_{tr} \Delta x$	$\sigma_{tr} \Delta y$		
	.01	1	100
.01	0.90		
1	0.83	0.64	
100	0.998	0.98	0.71

Table 5: Numerical Spectral Radii, BLD S_8 - S_4 - S_2 -DSA (WLA) Iteration, Optimized FP Scattering

$\sigma_{tr}\Delta x$	$\sigma_{tr}\Delta y$		
	.01	1	100
.01	1.48		
1	0.62	0.64	
100	0.97	0.98	0.71

Table 6: Numerical Spectral Radii, BLD S_8 - S_4 - S_2 -DSA-filter (WLA) Iteration, Optimized FP Scattering

$\sigma_{tr}\Delta x$	$\sigma_{tr}\Delta y$		
	.01	1	100
.01	0.74		
1	0.83	0.64	
100	0.99	0.98	0.71

4 Numerical Results

In order to confirm the Fourier analyses of the previous section, we use the transport code PERICLES, an unstructured mesh discrete ordinates code under development at Los Alamos National Laboratory (Wareing, 1999). For each calculation we use a rectangular mesh with as many elements as necessary or as computationally feasible to minimize leakage. In Tables 5 and 6 we list the numerically observed spectral radii from PERICLES for a BLD calculation with S_8 quadrature accelerated by the ANMG method without and with filtering, respectively. The numerical results compare well with the theoretical ones in Tables 3 and 4.

As a demonstration of the utility of ANMG acceleration in realistic calculations we apply it to a coupled electron-photon problem. The problem to be solved consists of a 30 mil \times 60 mil aluminum shield, on one side of which an isotropic, monoenergetic source of electrons is incident. The energy of the incident electrons is in the range 1-4 MeV. This problem was previously reported by Seltzer (Seltzer, 1979) and by Datta et al. (Datta, 1996). We divide the shield into a 20 \times 40 mesh of square elements, use an S_{12} Galerkin quadrature, and use CEPXS cross sections (Lorence, 1989) with 20 electron and 20 photon groups of uniform width with a cutoff energy of 50 keV. We also use linear discontinuous differencing of the continuous slowing down (CSD) operator. The calculated dose

Table 7: ANMG and DSA Performance, Electron-Photon Test Problem, LD-CSD Operator

Incident Energy [MeV]	Iterations, ANMG	Iterations, DSA	Inner CPU [s], ANMG	Inner CPU [s], DSA	Total CPU [s], ANMG	Total CPU [s], DSA
1	211	710	5403	14138	19517	27703
2	215	665	5501	13278	19569	26900
3	207	614	5226	12284	19094	25910
4	207	579	5238	11636	19124	25235

profile for 1 MeV incident electrons is shown in Figure 4. In Table 7 we report the timing results for this calculation with the unfiltered ANMG scheme and with DSA alone. The DSA and ANMG iterative methods are applied only to the within-group or “inner” iteration; neither method attempts to speed the calculation of group-to-group scattering. Thus, the most significant comparisons are total iterations and CPU time spent performing inner iterations. The table shows that although each ANMG iteration costs slightly more than a DSA iteration, it is still faster by a factor of 2 or 3. Overall run time was not reduced by as large a factor, because in this particular problem the downscattering calculation time is a major component of the total CPU time.

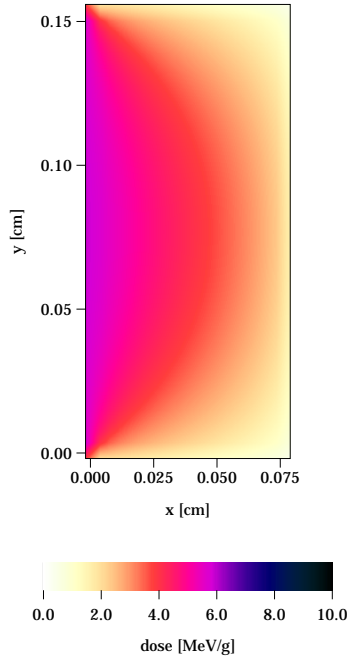


Figure 4: Dose in aluminum shield, 1 MeV incident electrons.

We have conducted other numerical tests that are not reported here. These tests include three-dimensional calculations of model problems and two-dimensional calculations of multimaterial problems. In all cases the ANMG scheme is more effective than DSA alone, and vastly more effective than simple source iteration, which is simply too slow to be of practical utility.

5 Conclusions

We have extended the angular multigrid method to multidimensional S_N calculations. Provided that the ANMG corrections are diffusively filtered or that the spatial cells are sufficiently thick, the ANMG scheme is stable and effective when scattering is highly forward-peaked. This has been shown by Fourier analyses of model problems, computations of model problems, and computations of realistic problems.

There are some areas of research that warrant further attention. The ANMG method makes use of diffusion operators for DSA and for filtering; the method could be improved if more effective or more easily solved diffusion operators were found. It seems likely that one could also eliminate the need for filtering if a combined angular and spatial multigrid were developed, since a sufficiently coarsened spatial mesh would not produce instabilities at high frequencies.

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